Anomaly at $\Delta_{\mathbf{k}}$ in the angle-resolved photoemission spectrum of dirty superconductors

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Elastic forward scattering can lead to an anomaly in the angle-resolved photoemission spectrum of the cuprate superconductors. Here we discuss how this anomaly can be used to provide a measurement of the superconducting gap $\Delta_{\mathbf{k}}$ for $\mathbf{k}$ values away from the Fermi surface.

In the search to understand the mechanism responsible for pairing in the cuprate high T_c superconductors, a key signature is thought to be the momentum dependence of the gap. A gap which has the simple $(\cos k_x - \cos k_y)$ dependence throughout the Brillouin zone would imply that the pairing arose from a near neighbor Cu-Cu interaction such as a superexchange coupling. Additional $\mathbf{k}$ dependence, involving higher $d_{x^2-y^2}$ harmonics, would imply a more extended spatial interaction[1], and some angle-resolved photoemission spectroscopy (ARPES) data on underdoped cuprates have indeed been used to suggest that the underdoped materials may have a longer range pairing[2]. Information on the gap function for values of $\mathbf{k}$ on the Fermi surface have been obtained from low temperature transport measurements [3], which probe the nodal regions, and from ARPES measurements[4]. While the peak at the quasiparticle energy $E(\mathbf{k})$ in the ARPES energy distribution function (EDC) can in principle be used to determine $\Delta_{\mathbf{k}}$ for $\mathbf{k}$ values away from the Fermi surface, this requires assuming a band structure and neglecting self-energy shifts. In addition, the EDC can be broad and asymmetric because of interactions, making the determination of the peak position uncertain. Here we discuss an alternative possibility for determining the $\mathbf{k}$ dependence of the gap away from the Fermi surface for general values of $\mathbf{k}$ based upon a structure in $A(\mathbf{k}, \omega)$ introduced by forward elastic scattering processes.

One expects that in $Bi_2Sr_2CaCu_2O_8$ (BSCCO) out-of-plane impurities or disorder will lead to forward elastic scattering[5]. A general discussion of the effect that such scattering can have on the ARPES spectrum was previously given[6, 7]. Here we will focus on one aspect of the scattering which leads to an anomalous structural feature in the ARPES spectral EDC at an energy equal to $\Delta_{\mathbf{k}}$. To illustrate the idea, we begin by considering just the effect of strong forward elastic scattering where the Nambu self-energies can be approximated by

$$\Sigma_0^{''}(\mathbf{k}, \omega) = -\Gamma_0(\mathbf{k}) \frac{|\omega|}{\sqrt{\omega^2 - \Delta_{\mathbf{k}}^2}} \qquad (1)$$

$$\Sigma_1^{''}(\mathbf{k}, \omega) = -\Gamma_0(\mathbf{k}) \frac{\Delta_{\mathbf{k}} \mathrm{sgn}\omega}{\sqrt{\omega^2 - \Delta_{\mathbf{k}}^2}} \qquad (2)$$

$$\Sigma_3^{''}(\mathbf{k}, \omega) \cong 0. \qquad (3)$$

The conditions for this approximation to be valid were discussed in [6]. Here $\Gamma_0(\mathbf{k})$ is the normal state scattering rate due to out-of-plane impurities. Note, that expressions (1) and (2) possess square-root divergences at the gap edge $\omega = \pm\Delta_{\mathbf{k}}$. Using these self-energies, the one-electron spectral weight can be written as [6, 8]

$$A(\mathbf{k}, \omega) = -\frac{1}{\pi} \mathrm{Im} \left\{ \frac{\omega Z(\mathbf{k}, \omega) + \epsilon_{\mathbf{k}}}{(\omega^2 - \Delta_{\mathbf{k}}^2) Z^2(\mathbf{k}, \omega) - \epsilon_{\mathbf{k}}^2} \right\} \qquad (4)$$

where $Z(\mathbf{k}, \omega) = 1 + i\Gamma_0(\mathbf{k}) \, \mathrm{sgn}\, \omega / \sqrt{\omega^2 - \Delta_{\mathbf{k}}^2}$. In the following we will set

$$\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - \mu \qquad (5)$$

with $t'/t = -0.35$ and $\mu/t = -1$, giving the Fermi surface shown in Fig 1. We will also assume for the purpose of illustration that

$$\Delta_{\mathbf{k}} = \frac{\Delta_0}{2}(\cos k_x - \cos k_y) \qquad (6)$$

with $\Delta_0 = 0.2t$.

Fig. 2(a) shows a plot of $A(\mathbf{k}, \omega)$ for several values of the normal state forward scattering rate $\Gamma_0(\mathbf{k})$ for $\mathbf{k} = (0.64\pi, 0)$ [the start of the A-cut shown in Fig. 1]. As expected, there is a broadened quasiparticle peak at $\omega = -\sqrt{\epsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}$. However, in addition there is a square-root anomaly as ω approaches $-\Delta_{\mathbf{k}}$. From eq. (4) one finds that for $\mathbf{k}$ away from the Fermi surface with $|\epsilon_{\mathbf{k}}| > \Delta_{\mathbf{k}}$,

$$A(\mathbf{k}, \omega \to -\Delta_{\mathbf{k}}) \simeq \frac{\Delta_{\mathbf{k}} \Gamma_0(\mathbf{k})}{\pi \epsilon_{\mathbf{k}}^2} \frac{1}{\sqrt{\omega^2 - \Delta_{\mathbf{k}}^2}} \qquad (7)$$

Thus, while the strength of the square-root anomaly caused by the forward scattering decreases as one goes deeper below the Fermi surface, the structure remains, and should be observable if the scattering rate $\Gamma_0(\mathbf{k})$ is sufficiently large.

In general, out-of-plane impurities will give rise to a scattering potential characterized by a finite range κ^{-1},
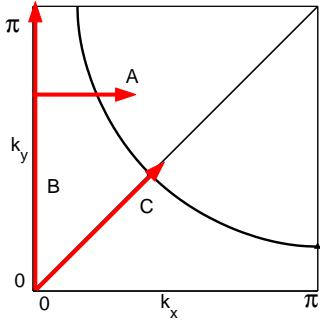
FIG. 1: Fermi surface in one quadrant of the first Brillouin zone for $t'/t = 0.35$ and $\mu/t = -1$ corresponding to a filling $n = .83$. Also shown are various momentum cuts A, B, and C for which EDC spectra are shown in Figures 3 and 4.
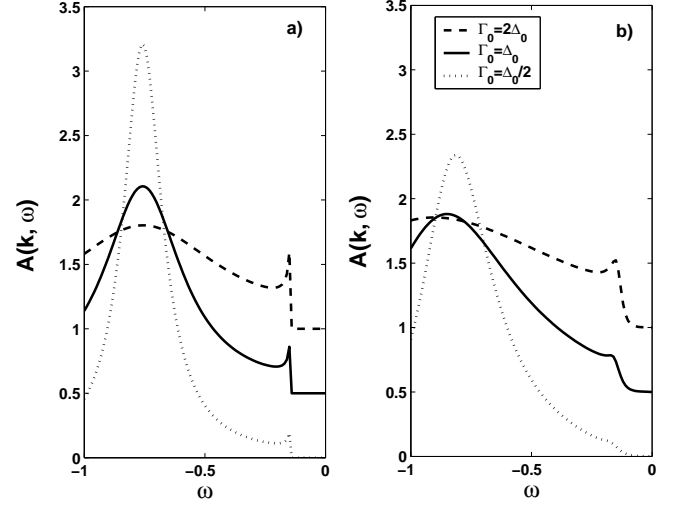

FIG. 2: a) Approximate spectral function $A(\mathbf{k}, \omega)$ from Eq (4) versus ω for $\mathbf{k} = (0.64\pi, 0)$ with $\Gamma_0 = 2\Delta_0$ (dashed curve), Δ_0 (solid curve) and $\Delta_0/2$ (dotted curve), with $\Delta_0 = 0.2t$. b) shows the numerical result obtained from the self-consistent Born approximation as described in Ref. [6], with $\kappa = 1$ and the same scattering rates. Curves are offset by 0.5 with respect to each other and ω is given in units of t.

and a more complete, self-consistent treatment of the self-energy due to impurity scattering is required. Here, we follow the approach taken in [6] in which a simple exponential scattering potential $V_0 e^{-\kappa r}$ was treated within a self-consistent Born approximation. In this case, the scattering strength depends upon both $\mathbf{k}$ and ω. For $\omega = -\Delta_{\mathbf{k}}$, the scattering strength is suppressed when $|\epsilon_{\mathbf{k}}|$ is greater than $\epsilon_\kappa \equiv v_F \kappa$ due to phase space restrictions. Nevertheless, as shown in Fig. 2(b), the anomaly continues to occur at $\omega = -\Delta_{\mathbf{k}}$, although the structure can be broadened somewhat. Here, we have set $\kappa = 1$, measured in inverse units of the Cu-Cu spacing, and chosen the strength of the out-of-plane impurity scattering potential and the impurity concentration to fix the normal state scattering rate Γ_0 equal to $2\Delta_0$, Δ_0, and $\Delta_0/2$.

In general, many-body interactions give rise to a gap function which depends upon both $\mathbf{k}$ and ω. However, at low temperatures when ω is equal to the real part of the gap at the gap edge i.e. $\Delta_{\mathbf{k}} = \text{Re}[\Delta(\mathbf{k}, \omega = \Delta_{\mathbf{k}})]$, the broadening due to inelastic scattering vanishes as T^3 [9] and the imaginary part of the gap is determined by elastic impurity scattering only, i.e. the anomaly at $\Delta_{\mathbf{k}}$ is stable against many-body interactions. Thus, out-of-plane forward impurity scattering gives rise to the anomaly and in-plane isotropic impurity scattering leads to only a small broadening for low energies near the Fermi level. In our units, a typical value for the broadening due to in-plane scattering is of order $.02t$, a typical value of the in-plane scattering estimated from fits to STM studies [10]. It is irrelevant for the anomaly at the gap edge and other features at higher binding energies.

In order to illustrate the type of behavior one is looking for, in Fig. 3 we have plotted $A(\mathbf{k}, \omega)$ versus ω for a set of $\mathbf{k}$ values taken along the A-cut shown in Fig. 1. Here, $\kappa = 1$ and results including a self-consistent Born approximation treatment of the forward scattering, together with an in-plane constant scattering rate of $0.02t$, are shown for $\Gamma_0 = 2\Delta_0$, Δ_0, and $\Delta_0/2$. In Fig. 3, the solid red curve follows the $\Delta_{\mathbf{k}}$ anomaly while the dashed red curve indicates the quasiparticle energy $-\sqrt{\epsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}$.

The various $A(\mathbf{k}, \omega)$ spectra are offset for the different $\mathbf{k}$ values which are taken at a momentum separation of $\Delta\mathbf{k} = 0.035$ along the A-cut shown in Fig. 1.

As seen, the strength of the anomaly [11] depends upon the out-of-plane impurity scattering rate Γ_0. For $\Gamma_0 \gtrsim \Delta_0$, there is a clear anomaly which occurs at $\omega = -\Delta_{\mathbf{k}}$. Here, we have taken $\Delta_{\mathbf{k}} = \frac{\Delta_0}{2}(\cos k_x - \cos k_y)$ for illustration. In general, the anomaly occurs at $\Delta_{\mathbf{k}} = \text{Re}[\Delta(\mathbf{k}, \omega = \Delta_{\mathbf{k}})]$ and the locus of this anomaly allows one to determine the $\mathbf{k}$-dependence of the gap for general values of $\mathbf{k}$.

Further results for $A(\mathbf{k}, \omega)$ taken along the three momentum cuts A, B, and C are illustrated in Fig. 4. Here $\kappa = 1$ and Γ_0 has been set to $2\Delta_0$. As before, the solid red curve gives the locus of $-\Delta_{\mathbf{k}}$, while the dashed red curve follows the broadened quasiparticle dispersion $-\sqrt{\epsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}$. As seen along the B cut, the strength of the gap anomaly decreases as $\Delta_{\mathbf{k}}$ decreases. It is also suppressed when $|\epsilon_{\mathbf{k}}| > \epsilon_\kappa$ due to phase space restrictions associated with the forward elastic scattering process.

In Fig. 5 we show $A(\mathbf{k}, \omega)$ at the M point $\mathbf{k} = (\pi, 0)$ for three different values of κ in order to illustrate the influence of the range of the scattering potential on the anomaly. A rough criterion for the appearance of the anomaly is that κ should become smaller than 1, which means that the range of the scattering potential should become larger than one lattice spacing of the CuO_2 planes. This is likely to be the case for out of plane impurities in the cuprates because of their poor screening.

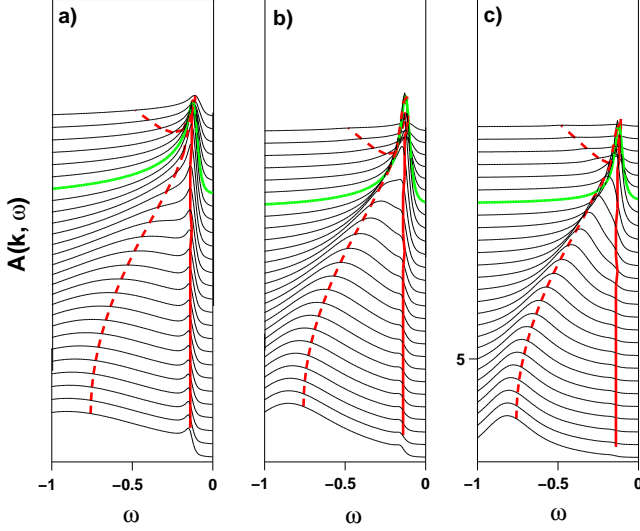In the foregoing analysis of the anomaly at $\Delta_{\mathbf{k}}$ we have

FIG. 3: a-c $A(\mathbf{k}, \omega)$ versus ω for $\mathbf{k}$ along the A cut shown in Figure 1 with a momentum separation $\Delta \mathbf{k} = 0.035$. These plots illustrate how the anomaly varies for $\kappa = 1$ and different values of the the scattering strength: (a)$\Gamma_0 = 2\Delta_0$; (b) $\Gamma_0 = \Delta_0$; (c) $\Gamma_0 = \Delta_0/2$, with $\Delta_0 = 0.2t$. The solid red curve indicates the $\Delta_\mathbf{k}$ anomaly, while the dashed red curve follows the quasiparticle dispersion. Fermi surface crossing spectra are colored green.
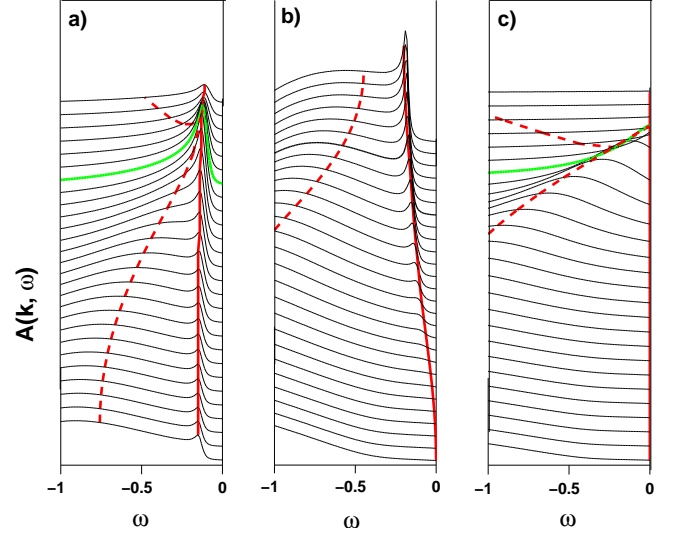
FIG. 4: a-c $A(\mathbf{k}, \omega)$ versus ω for $\mathbf{k}$ taken at intervals of $\delta\mathbf{k} = 0.0385, 0.12, 0.065$ along the A, B, C cuts shown in Figure 1, for $\Gamma_0 = 2\Delta_0$ and $\kappa = 1$. The solid red curve shows the locus of the anomaly which follows $\Delta_\mathbf{k} = \frac{\Delta_0}{2}(\cos k_x - \cos k_y)$. The dashed red curve follows the quasi-particle dispersion $-\sqrt{\epsilon_\mathbf{k}^2 + \Delta_\mathbf{k}^2}$, and the green curve represents the EDC at the Fermi surface crossing point.

restricted ourselves to the self-consistent Born approximation. It would be interesting to study effects beyond Born approximation, for example by employing the T-matrix approximation as in a recent work by Rieck et al [12], to see how this might affect the strength of the anomaly. The basic conclusion of our work, i.e. the existence and position of the anomaly at $\omega = -\Delta_\mathbf{k}$, will not be affected by the overall magnitude of the impurity potential, however (see, e.g. Eq. (7)). We leave the full calculation of the effect on ARPES of finite range scatterers of arbitrary potential for a future study.

In summary, the enhancement of the $\mathbf{k}$-dependent density of states at the gap edge $\omega = \pm\Delta_\mathbf{k}$ leads to an onset anomaly in $A(\mathbf{k}, \omega)$ due to forward elastic impurity scattering. The locus of this anomaly provides a direct measure of the $\mathbf{k}$-dependent gap $\Delta_\mathbf{k}$ at the gap edge. Strictly speaking, $\Delta_\mathbf{k} = \operatorname{Re}\Delta(\mathbf{k}, \omega = \Delta_\mathbf{k})$ where $\Delta(\mathbf{k}, \omega)$ is the complex $\mathbf{k}$ and ω-dependent gap function. As noted, at low temperatures with $\omega = \Delta_\mathbf{k}$, the imaginary part of the gap arising from inelastic scattering vanishes as $(T/\Delta_0)^3$ and in-plane elastic scattering leads to only a small imaginary contribution. Since out-of-plane forward elastic scattering gives rise to this anomaly, one would like to be able to control the number of surface defects, adjusting Γ_0 to obtain an optimal measurement. One possibility may be to purposely add impurities to the surface. It is also possible that older BSCCO samples may contain sufficient out of plane disorder to see the effect discussed here with modern energy and momentum resolution. Alternatively, as the experiment proceeds and the surface
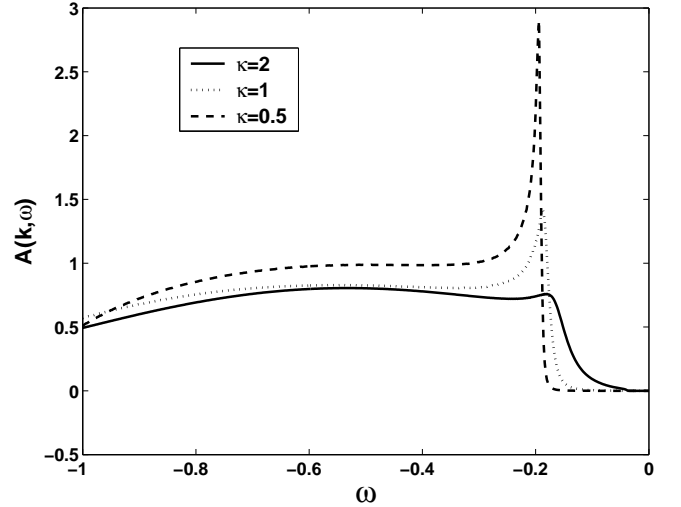

FIG. 5: $A(\mathbf{k}, \omega)$ versus ω for $\mathbf{k} = (\pi, 0)$ with $\Gamma_0 = 2\Delta_0$ and three different values of $\kappa = 2$ (solid curve), $\kappa = 1$ (dotted curve) and $\kappa = 0.5$ (dashed curve), with $\Delta_0 = 0.2t$.

gradually becomes contaminated, one may observe the development of this anomaly.

Acknowledgments

[1] The ω-dependence of the gap is also of interest since it reflects the retarded nature of the interaction. Here, we will focus on the question of the **k** dependence of the gap at a frequency equal to the gap.

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[11] It also depends upon κ and for **k** values deep inside the Fermi surface the size of the anomaly is suppressed by $(\epsilon_\kappa/|\epsilon_\mathbf{k}|)^5$ for the exponential potential we have used.

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